Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2025 – 11:23 AM EDT

PDB ID	:	7I2L
Title	:	Group deposition for crystallographic fragment screening of the NS5 RNA-dependent RNA polymerase from Dengue virus serotype 2 – Crystal structure of the NS5 RNA-dependent RNA polymerase from Dengue virus serotype 2 in complex with Z1627772104 (DNV2_NS5A-x0566)
Authors	:	Aschenbrenner, J.C.; Saini, M.; Chopra, A.; Marples, P.G.; Balcomb, B.H.; Lithgo, R.M.; Fearon, D.; von Delft, F.; Ruiz, F.X.; Arnold, E.
Deposited on	:	2025-03-06
Resolution	:	2.03 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

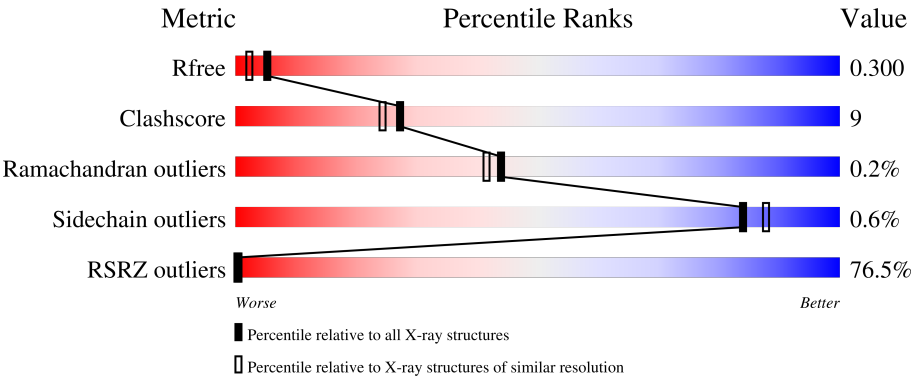
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	12358 (2.04-2.00)
Clashscore	180529	13897 (2.04-2.00)
Ramachandran outliers	177936	13770 (2.04-2.00)
Sidechain outliers	177891	13769 (2.04-2.00)
RSRZ outliers	164620	12358 (2.04-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	637	68% 72% 17% 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PO4	A	1007	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 4990 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NS5 RNA-dependent RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	566	4688	2951	839	864	34	0	7	0

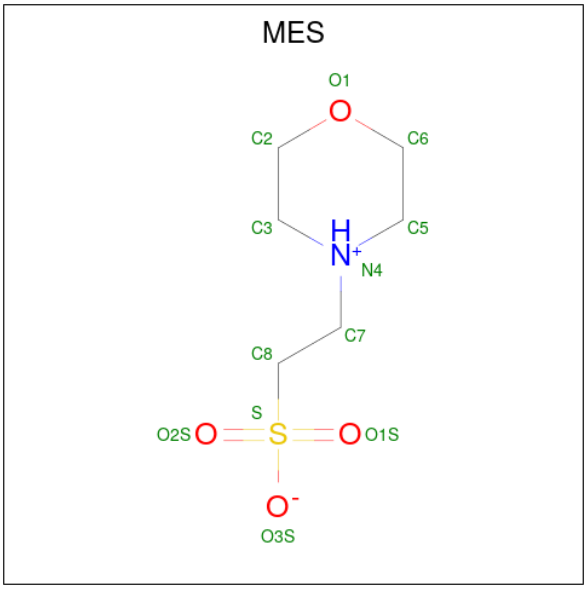
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	264	GLY	-	expression tag	UNP Q91H74
A	265	PRO	-	expression tag	UNP Q91H74

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

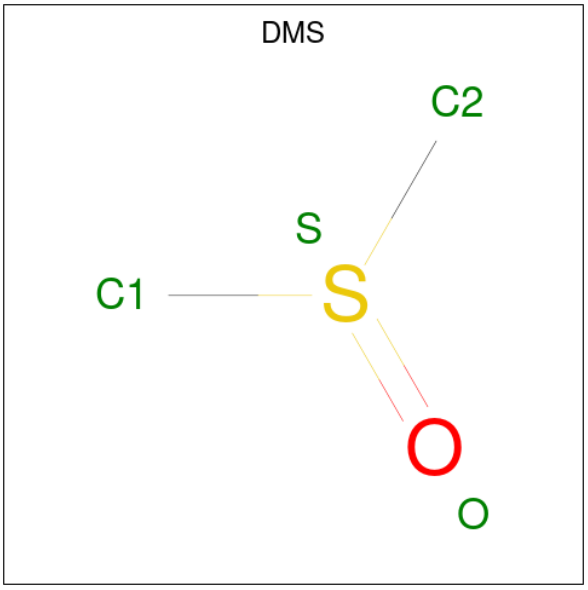
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	2	2	2	0	0

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



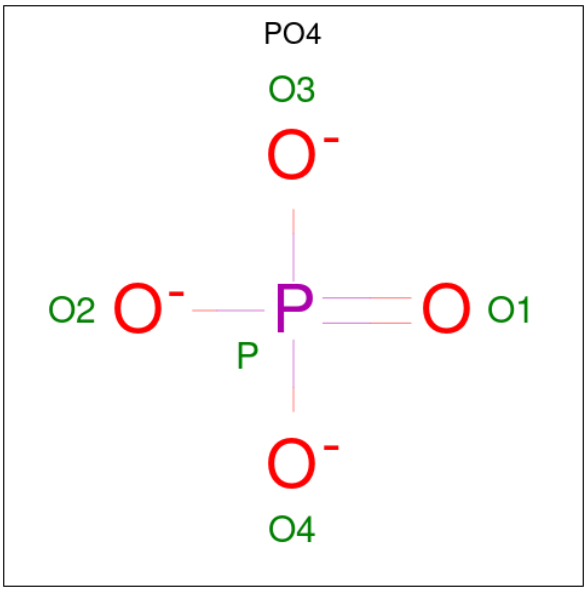
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	1
			24	12	2	8	2		

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



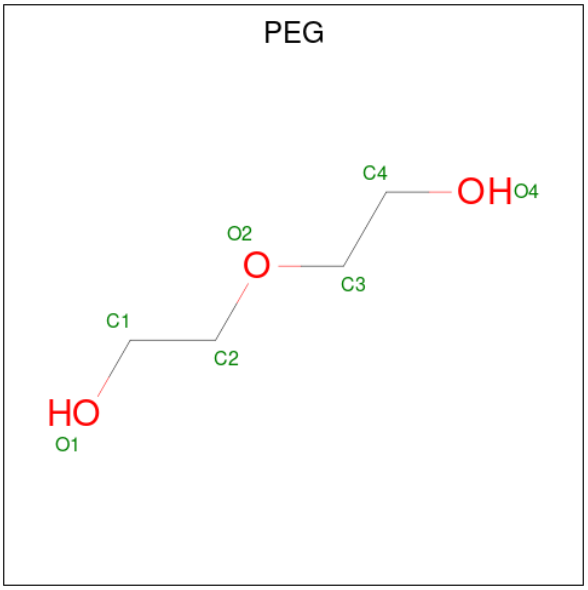
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	O	S		0	0
			4	2	1	1			
4	A	1	Total	C	O	S		0	0
			4	2	1	1			
4	A	1	Total	C	O	S		0	0
			4	2	1	1			

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O P 5 4 1	0	0
5	A	1	Total O P 5 4 1	0	0

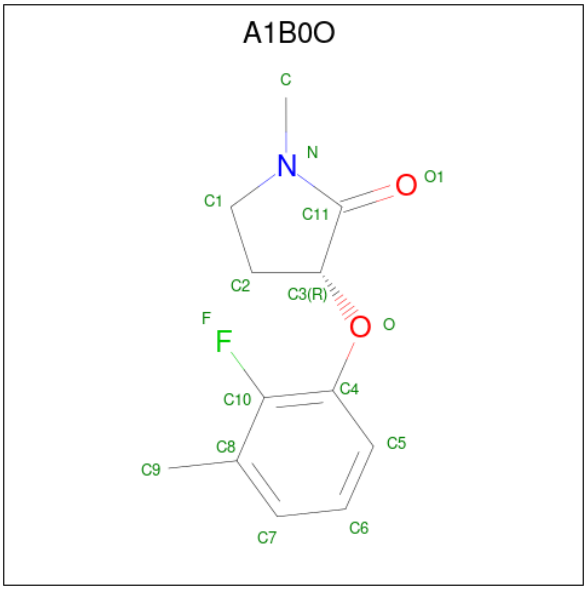
- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 4 3	0	0

- Molecule 7 is (3S)-3-(2-fluoro-3-methylphenoxy)-1-methylpyrrolidin-2-one (three-letter

code: A1B0O) (formula: $C_{12}H_{14}FNO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C F N O 16 12 1 1 2	0	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Cl 1 1	0	0

- Molecule 9 is water.

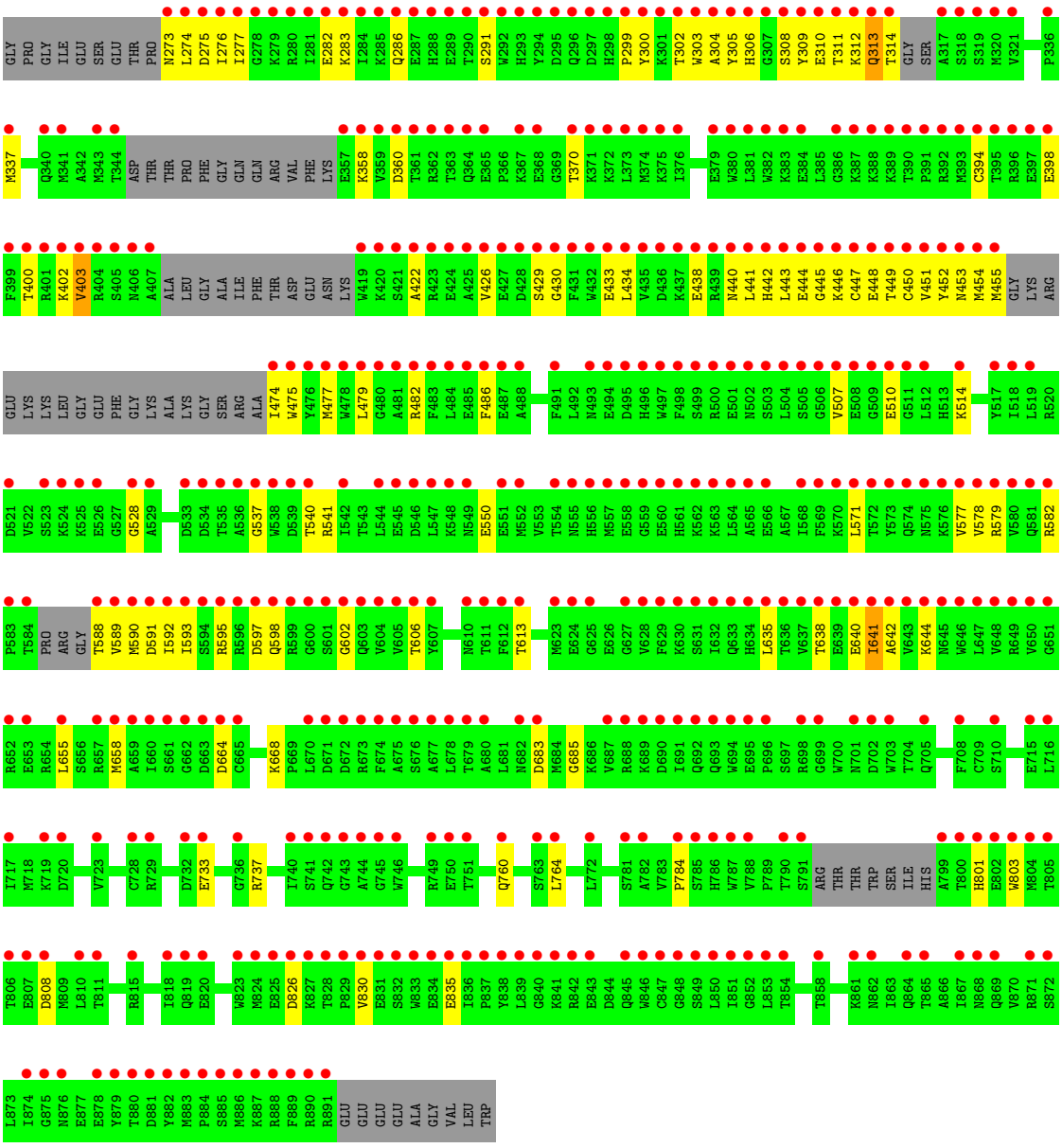
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	230	Total O 230 230	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: NS5 RNA-dependent RNA polymerase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	82.38Å 116.32Å 147.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.29 – 2.03 91.29 – 2.03	Depositor EDS
% Data completeness (in resolution range)	99.8 (91.29-2.03) 99.7 (91.29-2.03)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.03 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.200 , 0.243 0.280 , 0.300	Depositor DCC
R_{free} test set	2329 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	41.2	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 494.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.81	EDS
Total number of atoms	4990	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DMS, PO4, ZN, PEG, MES, CL, A1B0O

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.67	0/4793	0.74	0/6464

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	784	PRO	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4688	0	4580	83	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	24	0	26	1	0
4	A	12	0	18	1	0
5	A	10	0	0	2	0
6	A	7	0	10	0	0
7	A	16	0	0	0	0
8	A	1	0	0	0	0
9	A	230	0	0	4	0
All	All	4990	0	4634	85	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (85) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:MET:O	1:A:455:MET:CG	1.85	1.24
1:A:454:MET:O	1:A:455:MET:HG3	0.88	1.05
1:A:454:MET:C	1:A:455:MET:HG3	1.81	0.99
1:A:510:GLU:O	1:A:514:LYS:HG3	1.74	0.88
1:A:602:GLY:HA3	9:A:1204:HOH:O	1.72	0.88
1:A:453:ASN:ND2	1:A:579:ARG:HD2	1.94	0.83
1:A:438:GLU:HG3	1:A:449:THR:OG1	1.80	0.81
1:A:447:CYS:SG	1:A:450:CYS:HB2	2.21	0.81
1:A:304:ALA:O	1:A:593:ILE:HA	1.83	0.79
1:A:733:GLU:O	1:A:737:ARG:HG3	1.83	0.78
1:A:308:SER:HA	1:A:590:MET:O	1.84	0.77
1:A:400:THR:HG23	1:A:426:VAL:HG11	1.68	0.74
1:A:438:GLU:CG	1:A:449:THR:OG1	2.36	0.73
1:A:303:TRP:CE3	1:A:593:ILE:HD12	2.23	0.73
1:A:358:LYS:HG2	1:A:540:THR:HG21	1.70	0.73
1:A:664:ASP:OD1	5:A:1007:PO4:O4	2.09	0.71
1:A:442:HIS:O	1:A:445:GLY:N	2.19	0.70
1:A:303:TRP:CZ2	1:A:595:ARG:HD2	2.28	0.69
1:A:440:ASN:HA	1:A:443:LEU:HD12	1.75	0.68
1:A:664:ASP:OD1	5:A:1007:PO4:P	2.53	0.67
1:A:438:GLU:CD	1:A:449:THR:OG1	2.33	0.67
1:A:308:SER:HB3	1:A:589:VAL:HB	1.77	0.67
1:A:313:GLN:HG2	1:A:314:THR:H	1.63	0.62
1:A:358:LYS:HD3	1:A:537:GLY:HA3	1.80	0.62
1:A:274:LEU:HA	1:A:277:ILE:HG12	1.84	0.59
1:A:337:MET:HG2	9:A:1252:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:ASN:CG	1:A:579:ARG:HD2	2.23	0.58
1:A:273:ASN:N	1:A:275:ASP:OD1	2.37	0.57
1:A:422:ALA:HB1	1:A:479:LEU:HD22	1.85	0.57
4:A:1004:DMS:H12	9:A:1196:HOH:O	2.05	0.57
1:A:591:ASP:O	1:A:592:ILE:HD13	2.05	0.56
1:A:299:PRO:HD3	1:A:582:ARG:NH1	2.21	0.56
1:A:638:THR:O	1:A:641:ILE:HG23	2.06	0.56
1:A:507:VAL:O	1:A:510:GLU:HG2	2.07	0.55
1:A:311:THR:OG1	1:A:588:THR:HG22	2.07	0.54
1:A:602:GLY:O	1:A:606:THR:HB	2.10	0.51
1:A:283:LYS:HD2	1:A:448:GLU:HG2	1.92	0.50
1:A:507:VAL:C	1:A:510:GLU:HG2	2.31	0.50
1:A:400:THR:CG2	1:A:426:VAL:HG11	2.40	0.50
1:A:830:VAL:HG13	1:A:835:GLU:HB2	1.94	0.50
1:A:507:VAL:HA	1:A:510:GLU:HG3	1.94	0.49
1:A:398:GLU:O	1:A:402:LYS:HG3	2.12	0.49
1:A:400:THR:O	1:A:403:VAL:HG12	2.12	0.48
1:A:438:GLU:HA	1:A:441:LEU:HB2	1.95	0.48
1:A:438:GLU:O	1:A:441:LEU:HB2	2.14	0.48
1:A:444:GLU:HG2	1:A:446:LYS:HE2	1.96	0.47
1:A:589:VAL:HG23	1:A:589:VAL:O	2.14	0.47
1:A:429:SER:O	1:A:433:GLU:HG3	2.14	0.47
1:A:306:HIS:HB2	1:A:592:ILE:O	2.15	0.47
1:A:274:LEU:HA	1:A:277:ILE:CG1	2.45	0.46
1:A:305:TYR:CE1	1:A:591:ASP:OD1	2.69	0.46
1:A:635:LEU:HD23	1:A:640:GLU:HG2	1.96	0.45
1:A:302:THR:OG1	1:A:360:ASP:OD1	2.15	0.45
1:A:394:CYS:HB3	1:A:486:PHE:CE2	2.51	0.45
1:A:808:ASP:HB3	9:A:1240:HOH:O	2.16	0.45
1:A:291:SER:O	1:A:309:TYR:HA	2.17	0.45
1:A:655:LEU:HA	1:A:658:MET:HE2	1.99	0.45
1:A:597:ASP:O	1:A:598:GLN:HB2	2.17	0.45
1:A:582:ARG:O	1:A:588:THR:HA	2.17	0.44
1:A:302:THR:OG1	1:A:360:ASP:HA	2.18	0.44
1:A:430:GLY:O	1:A:434:LEU:HG	2.16	0.44
1:A:282:GLU:O	1:A:286:GLN:HG3	2.18	0.44
1:A:451:VAL:HG13	1:A:577:VAL:HG12	1.99	0.44
1:A:550:GLU:OE2	1:A:613:THR:OG1	2.29	0.43
1:A:640:GLU:HB3	1:A:644:LYS:NZ	2.34	0.43
1:A:826:ASP:OD1	1:A:826:ASP:C	2.56	0.43
1:A:592:ILE:O	1:A:592:ILE:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:TYR:HB2	1:A:578:VAL:HG22	2.00	0.42
1:A:528:GLY:O	1:A:668:LYS:HE3	2.18	0.42
1:A:450:CYS:C	1:A:477:MET:HE2	2.39	0.42
1:A:602:GLY:O	1:A:606:THR:CB	2.67	0.42
1:A:291:SER:HB3	1:A:310:GLU:H	1.84	0.42
1:A:801[B]:HIS:CD2	1:A:801[B]:HIS:H	2.37	0.42
1:A:299:PRO:HD2	1:A:300:TYR:CE2	2.54	0.42
1:A:370:THR:OG1	1:A:683:ASP:OD2	2.32	0.42
1:A:303:TRP:CD2	1:A:593:ILE:HD12	2.55	0.42
1:A:312:LYS:O	1:A:313:GLN:HB2	2.18	0.42
1:A:764:LEU:HD12	1:A:764:LEU:HA	1.83	0.42
1:A:474:ILE:HD12	1:A:474:ILE:N	2.35	0.41
1:A:641:ILE:HD13	1:A:642:ALA:N	2.33	0.41
3:A:1003[B]:MES:H32	3:A:1003[B]:MES:H81	1.91	0.41
1:A:276:ILE:HG23	1:A:571:LEU:HD22	2.03	0.41
1:A:541:ARG:HD2	1:A:685:GLY:O	2.21	0.41
1:A:760:GLN:NE2	1:A:803:TRP:O	2.54	0.40
1:A:452:TYR:HB3	1:A:475:TRP:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	559/637 (88%)	527 (94%)	31 (6%)	1 (0%)	44 41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	313	GLN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	505/554 (91%)	502 (99%)	3 (1%)	84 88

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	403	VAL
1	A	482	ARG
1	A	641	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	556	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	MES	A	1003[B]	-	12,12,12	0.71	0	15,16,16	0.29	0
5	PO4	A	1007	-	4,4,4	2.35	1 (25%)	6,6,6	0.77	0
3	MES	A	1003[A]	-	12,12,12	0.62	0	15,16,16	0.71	0
4	DMS	A	1004	-	3,3,3	0.44	0	3,3,3	0.28	0
4	DMS	A	1005	-	3,3,3	0.28	0	3,3,3	0.09	0
5	PO4	A	1008	-	4,4,4	0.67	0	6,6,6	0.49	0
6	PEG	A	1009	-	6,6,6	0.13	0	5,5,5	0.17	0
4	DMS	A	1006	-	3,3,3	0.17	0	3,3,3	0.42	0
7	A1B0O	A	1010	-	15,17,17	0.27	0	16,24,24	0.30	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MES	A	1003[A]	-	-	0/6/14/14	0/1/1/1
3	MES	A	1003[B]	-	-	3/6/14/14	0/1/1/1
7	A1B0O	A	1010	-	-	0/4/17/17	0/2/2/2
6	PEG	A	1009	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1007	PO4	P-O1	4.17	1.60	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1009	PEG	O2-C3-C4-O4
3	A	1003[B]	MES	C7-C8-S-O3S
3	A	1003[B]	MES	C7-C8-S-O1S
3	A	1003[B]	MES	C7-C8-S-O2S

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Mol	Chain	Res	Type	Atoms
6	A	1009	PEG	O1-C1-C2-O2

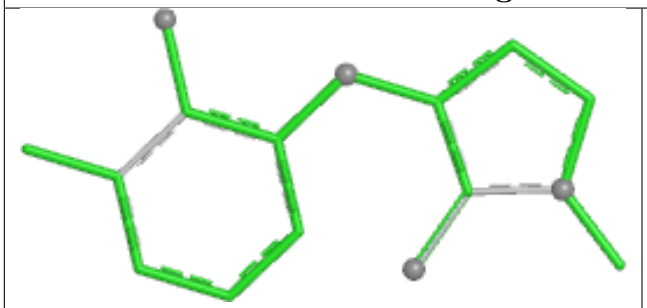
There are no ring outliers.

3 monomers are involved in 4 short contacts:

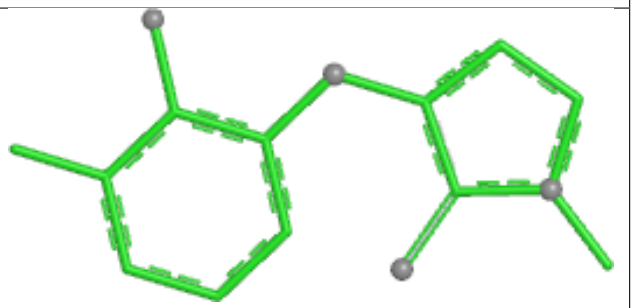
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1003[B]	MES	1	0
5	A	1007	PO4	2	0
4	A	1004	DMS	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

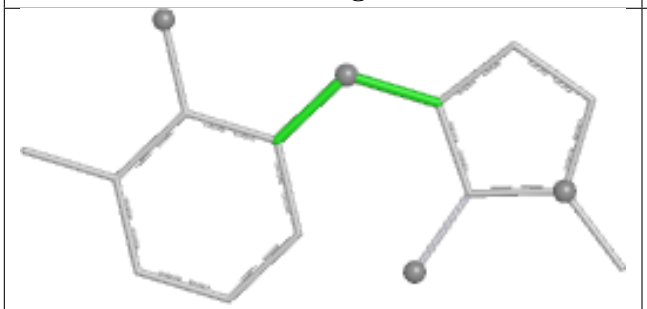
Ligand A1B0O A 1010



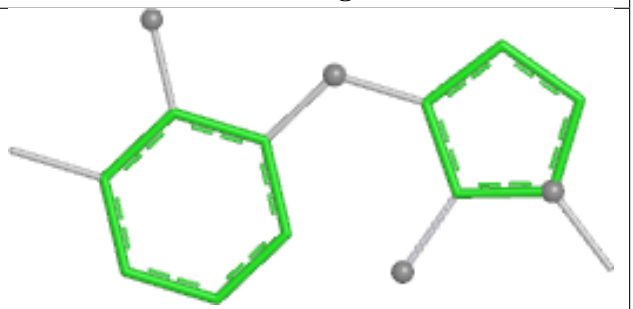
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	566/637 (88%)	6.23	433 (76%)	0	0	7, 39, 71, 147	261 (46%)

All (433) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	344	THR	23.6
1	A	364	GLN	20.1
1	A	287	GLU	18.9
1	A	274	LEU	18.5
1	A	281	ILE	18.2
1	A	275	ASP	17.8
1	A	403	VAL	17.3
1	A	600	GLY	17.1
1	A	425	ALA	16.5
1	A	284	ILE	16.5
1	A	276	ILE	16.1
1	A	889	PHE	15.9
1	A	308	SER	15.9
1	A	282	GLU	15.7
1	A	589	VAL	15.4
1	A	359	VAL	15.3
1	A	474	ILE	15.3
1	A	584	THR	14.9
1	A	431	PHE	14.7
1	A	407	ALA	14.3
1	A	435	VAL	14.3
1	A	289	GLU	14.2
1	A	426	VAL	14.2
1	A	888	ARG	14.0
1	A	363	THR	13.9
1	A	890	ARG	13.8
1	A	357	GLU	13.7

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Mol	Chain	Res	Type	RSRZ
1	A	294	TYR	13.7
1	A	278	GLY	13.7
1	A	441	LEU	13.6
1	A	280	ARG	13.4
1	A	305	TYR	13.4
1	A	648	VAL	13.4
1	A	291	SER	13.3
1	A	405	SER	13.3
1	A	518	ILE	13.3
1	A	434	LEU	13.3
1	A	277	ILE	13.2
1	A	742	GLN	13.1
1	A	592	ILE	13.0
1	A	593	ILE	13.0
1	A	650	VAL	12.9
1	A	601	SER	12.8
1	A	286	GLN	12.7
1	A	825	GLU	12.6
1	A	312	LYS	12.6
1	A	497	TRP	12.6
1	A	309	TYR	12.5
1	A	406	ASN	12.4
1	A	453	ASN	12.4
1	A	443	LEU	12.4
1	A	744	ALA	12.4
1	A	288	HIS	12.3
1	A	836	ILE	12.3
1	A	571	LEU	12.2
1	A	317	ALA	12.2
1	A	544	LEU	12.2
1	A	314	THR	12.2
1	A	481	ALA	12.2
1	A	428	ASP	12.1
1	A	404	ARG	12.1
1	A	646	TRP	12.0
1	A	292	TRP	11.9
1	A	432	TRP	11.8
1	A	603	GLN	11.8
1	A	641	ILE	11.8
1	A	604	VAL	11.8
1	A	887	LYS	11.7
1	A	745	GLY	11.7

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Mol	Chain	Res	Type	RSRZ
1	A	643	VAL	11.6
1	A	687	VAL	11.6
1	A	886	MET	11.6
1	A	649	ARG	11.6
1	A	283	LYS	11.6
1	A	476	TYR	11.5
1	A	399	PHE	11.5
1	A	511	GLY	11.5
1	A	885	SER	11.5
1	A	478	TRP	11.4
1	A	475	TRP	11.4
1	A	307	GLY	11.3
1	A	423	ARG	11.3
1	A	519	LEU	11.3
1	A	651	GLY	11.2
1	A	582	ARG	11.2
1	A	763[A]	SER	11.2
1	A	602	GLY	11.2
1	A	302	THR	11.1
1	A	311	THR	11.1
1	A	358	LYS	11.0
1	A	493	ASN	11.0
1	A	438	GLU	10.9
1	A	572	THR	10.8
1	A	781	SER	10.8
1	A	483	PHE	10.8
1	A	480	GLY	10.7
1	A	583	PRO	10.7
1	A	637	VAL	10.7
1	A	801[A]	HIS	10.6
1	A	290	THR	10.6
1	A	400	THR	10.5
1	A	577	VAL	10.5
1	A	512[A]	LEU	10.5
1	A	422	ALA	10.4
1	A	631	SER	10.4
1	A	563	LYS	10.4
1	A	430	GLY	10.3
1	A	558	GLU	10.3
1	A	498	PHE	10.3
1	A	578	VAL	10.2
1	A	421	SER	10.2

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Mol	Chain	Res	Type	RSRZ
1	A	303	TRP	10.2
1	A	846	TRP	10.2
1	A	636	THR	10.2
1	A	383	LYS	10.1
1	A	419	TRP	10.1
1	A	479	LEU	10.1
1	A	891	ARG	10.1
1	A	833	TRP	10.0
1	A	285	LYS	10.0
1	A	647	LEU	10.0
1	A	402	LYS	10.0
1	A	791	SER	9.9
1	A	452	TYR	9.9
1	A	635	LEU	9.9
1	A	645	ASN	9.9
1	A	642	ALA	9.9
1	A	514	LYS	9.7
1	A	719[A]	LYS	9.7
1	A	785[A]	SER	9.6
1	A	420	LYS	9.6
1	A	433	GLU	9.6
1	A	437	LYS	9.6
1	A	837	PRO	9.6
1	A	751	THR	9.5
1	A	573	TYR	9.5
1	A	361	THR	9.5
1	A	540	THR	9.5
1	A	799	ALA	9.5
1	A	606	THR	9.5
1	A	655	LEU	9.4
1	A	678	LEU	9.4
1	A	477	MET	9.4
1	A	362	ARG	9.4
1	A	864[A]	GLN	9.4
1	A	424	GLU	9.4
1	A	632	ILE	9.3
1	A	273	ASN	9.2
1	A	657	ARG	9.2
1	A	835	GLU	9.2
1	A	449	THR	9.1
1	A	293	HIS	9.1
1	A	499	SER	9.1

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Mol	Chain	Res	Type	RSRZ
1	A	741[A]	SER	9.0
1	A	484	LEU	9.0
1	A	708	PHE	9.0
1	A	851	ILE	9.0
1	A	539	ASP	9.0
1	A	300	TYR	9.0
1	A	679	THR	8.9
1	A	576	LYS	8.9
1	A	395	THR	8.9
1	A	790	THR	8.8
1	A	506	GLY	8.8
1	A	337	MET	8.7
1	A	360	ASP	8.7
1	A	304	ALA	8.7
1	A	659	ALA	8.7
1	A	675	ALA	8.7
1	A	501	GLU	8.7
1	A	694	TRP	8.7
1	A	429	SER	8.6
1	A	279	LYS	8.6
1	A	575	ASN	8.6
1	A	580	VAL	8.6
1	A	504	LEU	8.6
1	A	638	THR	8.6
1	A	538	TRP	8.6
1	A	442	HIS	8.5
1	A	505	SER	8.5
1	A	581	GLN	8.4
1	A	548	LYS	8.4
1	A	546	ASP	8.3
1	A	691	ILE	8.3
1	A	556	HIS	8.3
1	A	447	CYS	8.2
1	A	591	ASP	8.2
1	A	436	ASP	8.2
1	A	629	PHE	8.2
1	A	450	CYS	8.1
1	A	507	VAL	8.1
1	A	640	GLU	8.1
1	A	850	LEU	8.1
1	A	594	SER	8.1
1	A	455	MET	8.1

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Mol	Chain	Res	Type	RSRZ
1	A	839	LEU	8.1
1	A	298	HIS	8.1
1	A	849	SER	8.1
1	A	676	SER	8.0
1	A	644	LYS	8.0
1	A	536	ALA	8.0
1	A	800	THR	8.0
1	A	677	ALA	7.9
1	A	296	GLN	7.9
1	A	633	GLN	7.9
1	A	688	ARG	7.9
1	A	834	GLU	7.9
1	A	693	GLN	7.8
1	A	876	ASN	7.8
1	A	295	ASP	7.8
1	A	660	ILE	7.8
1	A	788	VAL	7.7
1	A	808	ASP	7.7
1	A	838	TYR	7.7
1	A	545	GLU	7.7
1	A	652	ARG	7.7
1	A	852	GLY	7.6
1	A	365	GLU	7.6
1	A	701	ASN	7.6
1	A	301	LYS	7.6
1	A	427	GLU	7.6
1	A	627	GLY	7.5
1	A	487	GLU	7.5
1	A	310	GLU	7.4
1	A	639	GLU	7.4
1	A	750	GLU	7.4
1	A	807	GLU	7.4
1	A	588	THR	7.4
1	A	448	GLU	7.3
1	A	705	GLN	7.3
1	A	454	MET	7.3
1	A	661	SER	7.3
1	A	596	ARG	7.3
1	A	396	ARG	7.3
1	A	597	ASP	7.3
1	A	673	ARG	7.2
1	A	692	GLN	7.2

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Mol	Chain	Res	Type	RSRZ
1	A	595	ARG	7.1
1	A	318	SER	7.1
1	A	658	MET	7.0
1	A	535	THR	6.9
1	A	306	HIS	6.9
1	A	786	HIS	6.9
1	A	551	GLU	6.9
1	A	299	PRO	6.9
1	A	566	GLU	6.9
1	A	882	TYR	6.9
1	A	440	ASN	6.8
1	A	401	ARG	6.8
1	A	482	ARG	6.8
1	A	398	GLU	6.8
1	A	510	GLU	6.8
1	A	663	ASP	6.8
1	A	842	ARG	6.7
1	A	590	MET	6.7
1	A	746	TRP	6.7
1	A	537	GLY	6.6
1	A	806	THR	6.6
1	A	574	GLN	6.6
1	A	503	SER	6.5
1	A	500	ARG	6.5
1	A	446	LYS	6.5
1	A	502	ASN	6.5
1	A	562	LYS	6.5
1	A	880	THR	6.5
1	A	840	GLY	6.4
1	A	313	GLN	6.4
1	A	634	HIS	6.4
1	A	672	ASP	6.3
1	A	579	ARG	6.3
1	A	749	ARG	6.3
1	A	451	VAL	6.3
1	A	495	ASP	6.3
1	A	674	PHE	6.2
1	A	393	MET	6.2
1	A	802	GLU	6.2
1	A	854	THR	6.2
1	A	445	GLY	6.1
1	A	319	SER	6.1

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Mol	Chain	Res	Type	RSRZ
1	A	534	ASP	6.1
1	A	743	GLY	6.1
1	A	717	ILE	6.1
1	A	552	MET	6.1
1	A	695	GLU	6.0
1	A	367	LYS	6.0
1	A	570	LYS	6.0
1	A	321	VAL	5.9
1	A	861	LYS	5.9
1	A	804	MET	5.9
1	A	397	GLU	5.8
1	A	699	GLY	5.8
1	A	878	GLU	5.8
1	A	496	HIS	5.8
1	A	858	THR	5.8
1	A	524	LYS	5.7
1	A	815	ARG	5.7
1	A	689	LYS	5.6
1	A	494	GLU	5.6
1	A	828	THR	5.6
1	A	564	LEU	5.6
1	A	372	LYS	5.6
1	A	716	LEU	5.6
1	A	486	PHE	5.5
1	A	485	GLU	5.5
1	A	630	LYS	5.4
1	A	555	ASN	5.3
1	A	690	ASP	5.3
1	A	881	ASP	5.3
1	A	371	LYS	5.3
1	A	831	GLU	5.2
1	A	368	GLU	5.2
1	A	845	GLN	5.2
1	A	625	GLY	5.2
1	A	820	GLU	5.1
1	A	841	LYS	5.1
1	A	444	GLU	5.1
1	A	375	LYS	5.0
1	A	703	TRP	4.9
1	A	653	GLU	4.8
1	A	843	GLU	4.8
1	A	559	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	883	MET	4.7
1	A	379	GLU	4.7
1	A	811	THR	4.7
1	A	569	PHE	4.7
1	A	680	ALA	4.7
1	A	376	ILE	4.6
1	A	764	LEU	4.6
1	A	827	LYS	4.6
1	A	698	ARG	4.5
1	A	819	GLN	4.5
1	A	664	ASP	4.4
1	A	702	ASP	4.4
1	A	389	LYS	4.4
1	A	394	CYS	4.4
1	A	390	THR	4.3
1	A	683	ASP	4.3
1	A	565	ALA	4.3
1	A	340	GLN	4.3
1	A	488	ALA	4.3
1	A	874	ILE	4.3
1	A	508	GLU	4.3
1	A	392	ARG	4.3
1	A	561	HIS	4.2
1	A	740	ILE	4.2
1	A	297	ASP	4.2
1	A	818	ILE	4.2
1	A	628	VAL	4.1
1	A	387	LYS	4.0
1	A	784	PRO	3.9
1	A	439	ARG	3.9
1	A	542	ILE	3.8
1	A	830	VAL	3.8
1	A	607	TYR	3.8
1	A	624	GLU	3.8
1	A	670	LEU	3.7
1	A	610	ASN	3.7
1	A	320	MET	3.7
1	A	343	MET	3.7
1	A	853	LEU	3.7
1	A	729	ARG	3.7
1	A	760	GLN	3.6
1	A	868	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	715	GLU	3.6
1	A	823	TRP	3.6
1	A	568	ILE	3.6
1	A	611	THR	3.5
1	A	720	ASP	3.5
1	A	867	ILE	3.5
1	A	529	ALA	3.4
1	A	381	LEU	3.4
1	A	526	GLU	3.4
1	A	865	THR	3.4
1	A	879	TYR	3.3
1	A	872	SER	3.3
1	A	336	PRO	3.2
1	A	521	ASP	3.2
1	A	549	ASN	3.2
1	A	805	THR	3.1
1	A	391	PRO	3.1
1	A	373	LEU	3.1
1	A	875	GLY	3.1
1	A	723	VAL	3.1
1	A	803	TRP	3.0
1	A	696	PRO	3.0
1	A	662	GLY	3.0
1	A	848	GLY	2.9
1	A	826	ASP	2.9
1	A	598	GLN	2.9
1	A	832	SER	2.9
1	A	370	THR	2.8
1	A	862	ASN	2.8
1	A	732	ASP	2.8
1	A	386	GLY	2.7
1	A	829	PRO	2.7
1	A	599	ARG	2.7
1	A	733	GLU	2.7
1	A	623	MET	2.6
1	A	523	SER	2.6
1	A	557	MET	2.6
1	A	665	CYS	2.6
1	A	560	GLU	2.6
1	A	772	LEU	2.5
1	A	554	THR	2.5
1	A	782	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	533	ASP	2.4
1	A	671	ASP	2.4
1	A	388	LYS	2.4
1	A	491	PHE	2.4
1	A	869	GLN	2.4
1	A	380	TRP	2.4
1	A	847	CYS	2.3
1	A	341	MET	2.3
1	A	517	TYR	2.3
1	A	810	LEU	2.3
1	A	374	MET	2.3
1	A	547	LEU	2.3
1	A	824	MET	2.3
1	A	605	VAL	2.2
1	A	525	LYS	2.2
1	A	736	GLY	2.2
1	A	682	ASN	2.2
1	A	871	ARG	2.2
1	A	787	TRP	2.2
1	A	528	GLY	2.2
1	A	728	CYS	2.2
1	A	612	PHE	2.1
1	A	613	THR	2.1
1	A	884	PRO	2.1
1	A	382	TRP	2.1
1	A	384	GLU	2.1
1	A	710	SER	2.1
1	A	509	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

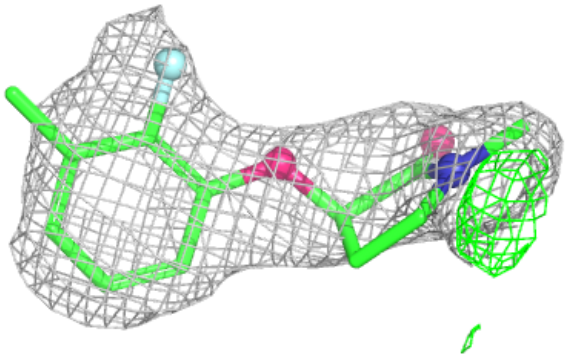
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

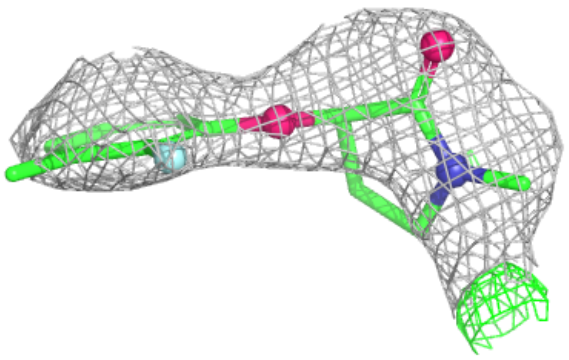
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PO4	A	1007	5/5	0.70	0.19	53,56,61,86	0
5	PO4	A	1008	5/5	0.72	0.19	111,118,123,131	0
6	PEG	A	1009	7/7	0.73	0.22	73,76,82,83	0
7	A1B0O	A	1010	16/16	0.77	0.23	37,38,41,41	16
4	DMS	A	1005	4/4	0.81	0.20	93,104,108,111	0
4	DMS	A	1006	4/4	0.91	0.20	67,68,72,76	0
3	MES	A	1003[A]	12/12	0.95	0.24	15,19,21,21	12
3	MES	A	1003[B]	12/12	0.95	0.24	477,485,528,530	12
4	DMS	A	1004	4/4	0.95	0.23	52,57,60,61	0
8	CL	A	1011	1/1	0.95	0.16	26,26,26,26	1
2	ZN	A	1002	1/1	0.98	0.07	61,61,61,61	0
2	ZN	A	1001	1/1	1.00	0.04	30,30,30,30	0

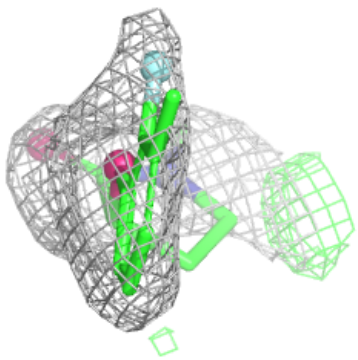
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around A1B0O A 1010:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.